

1,4-Ethanonaphtho(1,8-ef)-1,4-diazepine, 2,3-dihydro-
59950-41-3 | DTXSID40208664

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 126 °C

Global applicability domain: Inside

Local applicability domain index: 5.77e-01

Confidence level: 5.34e-01

Nearest Neighbors from the Training Set

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1,4-Diphenylpiperazine

Measured: 165

Predicted: 150

Image not found

Mebhydrolin

Measured: 95.0

Predicted: 105

Image not found

Benzo[c]cinnoline

Measured: 158

Predicted: 141

Image not found

Bamipine

Measured: 115

Predicted: 117

Image not found

Ethopropazine

Measured: 64.5

Predicted: 96.3